"Ambient MS and Direct to MS: Strategies for Quantitation" – Ambient Sampling and Ionization Interest Group

Presiders: Asher Newsome (Smithsonian Institution) German Gomez-Rios (Restek Corporation)

3-minute lightning talks selected from in-person posters: Tara Maser, Western Michigan University Allix Coon, University at Albany SUNY Changtong Hao, Advion Martin Kaufmann, Queen's University Shruthi Perna, Middle Tennessee State University Alena Bensussan, University of Texas-Austin Bettina Streckenbach, ETH Zurich Saquib Rahman, Purdue

To maximize available time, audience questions were deferred to post-workshop discussion with lightning talk speakers.

Panel on quantitation:

Robert Cody, JEOL Sylwia Stopka, Brigham and Women's Hospital/Harvard Medical School Anthoney Midey, Waters Patrick Fedick, Naval Air Warfare Center Weapons Division Margot De Spiegeleer, University of Ghent

The ease and approachability of ambient ionization and direct to MS sources have made them popular methods for qualitative analysis since the mid-2000s, but the operational elements that allow speed and minimal-to-no sample preparation are often at odds with the requirements for quantitation. At ASMS 2019, workshop attendees responded to a poll by rating "quantitative capabilities" and "reproducibility" as the top challenges in ambient ionization. Having discussed reproducibility (and lack of reproducibility) with short, virtual talks at the 2020 Reboot, this year we will host a panel of experts with hands-on experience to discuss challenges and strategies for quantitation with various sampling and ionization methods and analytes... The workshop aims to encourage audience participation and presentations from new investigators, postdocs, and graduate students with a balanced perspective from inside and outside academia.

Major panel discussion points:

DART ionization is affected by the turbulence barrier in transfer from atmospheric pressure to the MS vacuum.

DESI and DESI imaging have the ability to add standards to the desorbing solvent. Spraybased methods are able to use isotopically-labeled standards, which are relatively cheap. LAESI and LA-REIMS are subject to laser shot-to-shot variation, and efficient collection of the desorption plume is key. REIMS is subject to matrix effects.

The conespray configuration of a paperspray source is most affected by reproducibility in construction.

Sample transfer from the desorption point to the MS is improved by surrounding the source with a conductance chamber.

Decoupling desorption from ionization may allow more reproducible performance.

Reproducibility is unavoidably entwined with quantitation. What is an appropriate relative standard deviation figure for quantitation with ambient methods?

All quantitation methods with ambient sources require validation. LCMS is a reliable source of standardization, though other good knowns are possible.

Sample preparation technologies can increase performance.

Though it can be challenging, there is no shortage of ambient ionization literature describing quantitation.

Other business:

Celebration of new status as interest group.

Workshop extended for 15 minutes to compensate for late-running ASMS business meeting. Call for co-organizer to join German at ASMS 2022 and organize with new person in 2023. Headcount of in-person attendees of approximately 50 (with unknown number of virtual attendees) judged proportional to 40% live attendance to full ASMS conference compared to 2019.